

Analysis of Gasoline Negative-Valve-Overlap Fueling via Dump Sampling

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ABSTRACT

Negative valve overlap (NVO) is an operating mode that enables efficient, low-temperature gasoline combustion in automotive engines. In addition to retaining a large fraction of residuals, NVO operation also enables partial fuel injection during the recompression period as a means of enhancing and controlling main combustion. Thermal effects of NVO fueling on main combustion are well understood, but chemical effects of the products of NVO reactions remain uncertain. To address this topic, we have fabricated a dump valve that extracts a large fraction of cylinder charge at intake valve closing (IVC), yielding a representative sample of NVO products mixed with intake air. Sample composition is determined by gas chromatography. Results from a sweep of NVO start-of-injection (SOI) timings show that concentrations of the reactive species acetylene and hydrogen rise to several hundred parts-per-million as NVO SOI is retarded toward top center of NVO. Since experiments have previously demonstrated that low concentrations of acetylene seeded into the intake flow advance combustion phasing, the current results support the conclusion that NVO fueling can chemically enhance main combustion. This conclusion is further strengthened by a one-dimensional chemical kinetics simulation of main combustion that uses measured compositions as initial conditions at IVC. Comparing early and late NVO SOI, the model predicts that the hydrogen and acetylene produced by late NVO injection significantly advance the phasing of main combustion.

CITATION: Steeper, R. and Davisson, M., "Analysis of Gasoline Negative-Valve-Overlap Fueling via Dump Sampling," *SAE Int. J. Engines* 7(2):2014, doi:10.4271/2014-01-1273.

INTRODUCTION

The relentless drive for cleaner and more efficient engines has pushed research toward low-temperature gasoline combustion (LTGC) strategies that offer hope of achieving mandated ultra-low engine-out emissions. Such strategies often make use of auto-ignition to avoid high-temperature flames associated with spark ignition. However, this approach makes initiating and controlling LTGC a difficult challenge, especially during part-load operation.

Negative valve overlap (NVO), illustrated in the engine cycle of [Figure 1](#), is a well-known approach for gaining control of LTGC on a cycle-by-cycle timescale [1,2,3]. Several mechanisms contribute to the strategy. First, NVO can retain a large volume of residual gases for both thermal and dilution control of subsequent main combustion. Secondly, a variable fraction of each cycle's fuel can be injected during NVO's recompression period. Exothermal reaction of the NVO fuel elevates charge temperature further, contributing to the thermal control of main combustion. But depending on when and how much fuel is injected, NVO fueling can also produce reformed species that are carried over to chemically enhance main combustion.

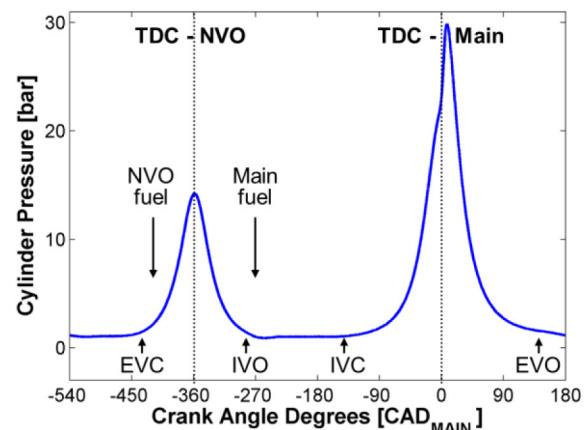


Figure 1. Typical pressure trace for fired NVO LTGC showing NVO and main portions of the cycle. Valve events are labeled, e.g., EVC = exhaust valve open, IVO = intake valve open, etc. Axis label CAD_{MAIN} = crank angle degrees after top dead center (TDC) of main compression. In later figures, the term CAD_{NVO} (CAD after TDC of NVO) is also used when more convenient.



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Many investigators [4,5,6,7,8,9,10,11,12,13,14] have examined *thermal effects* of NVO fueling on main combustion. In these studies, lean and near-stoichiometric conditions during NVO are typically selected to achieve high NVO combustion efficiencies that maximize thermal effects. Experiments designed to isolate *chemical effects* of NVO fueling are rarer [1,3,8,10,15,16,17,18]. Based on model predictions using a highly reduced reaction mechanism, Koopmans, et al. [1] discussed the role of NVO reaction intermediates on main combustion, but without many details of species concentrations. A pair of papers from Aroonsrisopon, Waldman, et al. [8,10] also acknowledged the role of NVO chemical effects. Chemistry modeling in these studies used a skeletal kinetic mechanism to predict significant NVO production of the reformed products ethylene and formaldehyde under high NVO fuel-loading conditions. There have been relatively few attempts to experimentally measure NVO product species. Three such investigations [15,16,17] are discussed in relation to the current research in the Gas Sampling Results section. In spite of these research efforts, fundamental details of chemical enhancement of main combustion due to NVO fueling remain uncertain.

Prior experiments in our lab addressed the issue of thermal and chemical effects of NVO fueling [19]. In those experiments a small fraction of total fuel was injected during NVO and the resulting main combustion phasing was measured. Notably, we found a distinct difference between early and late NVO fuel injection. Fuel injected early reacted relatively completely during NVO, elevating charge temperatures and advancing main combustion phasing. In contrast, fuel injected late during NVO reacted less completely, i.e., produced less heat during NVO, but it still advanced main combustion as much or more than early NVO injection. From this, we concluded that carry-over chemical species played an important role in the late NVO injection experiments. In optical experiments, we observed that late NVO fuel injection wetted the piston top, creating pool fires with conspicuous sooty flames - suggesting that the carry-over species are likely products of localized rich combustion.

Further experiments identified acetylene as a likely candidate species, examining its chemical effects via seeding experiments, where NVO fuel injection was replaced by a flow of acetylene into the intake air [20]. In that study, acetylene concentrations of 600 to 2300 ppm were found to advance main combustion phasing and elevate peak heat-release rates. The goal of the current work is to enhance understanding of NVO chemical effects by directly measuring the composition of products of NVO fueling.

APPROACH

Gas-Sampling System

Traditionally, cylinder gas sampling has relied on mini-sampling valves to extract small-volume samples that are rapidly quenched to provide time-resolved details of cylinder contents

[15,16,21,22,23]. But the mini-samples capture only a small fraction of cylinder contents, and the external quenching process can introduce uncertainty. In contrast, several researchers have developed full-cylinder sampling devices that capture a large fraction of cylinder contents [17,24,25,26]. In the current work, we pursue this approach by developing a dump valve that takes advantage of several characteristics of NVO engine operation. First, quenching of reactions occurs naturally as the NVO products are mixed with intake air, so no dilution gas flows in the sampling system are necessary. And there is no need to control the rate of quenching since we are interested only in reactive species that persist long enough in the cycle to influence main ignition and combustion. Extraction can conveniently begin at intake valve closing (IVC) when composition is fixed, pressure is low, and piston motion assists the extraction. Finally, the sampling valve can remain open for a relatively long period (IVC to EVO) allowing a voluminous sample to be captured using a system built from commonly available hardware.

The custom dump valve illustrated in [Figure 2](#) was designed and fabricated to fit in a conventional 14-mm threaded spark-plug port. The design mimics conventional engine valve geometry but with a scaled-down head diameter of 8 mm and lift of 3.2 mm. An automotive valve spring and retainer sit at the top of the valve stem next to a 3/16-inch Swagelok fitting providing passage for sample gases. A commercial, low-voltage solenoid at the top of the assembly is capable of actuating the valve in 4 ms (4 ms to open, and 4 ms to close). The dump-valve geometry maximizes sample flow while minimizing dead volume. All parts are designed to seal both vacuum and elevated pressures while tolerating brief exhaust-gas, and steady engine-block, temperatures. Comparing motored pressure traces with and without the valve installed indicates that the leak rate through the valve is insignificant compared to, for example, engine ring blowby.

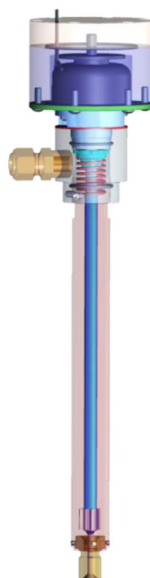


Figure 2. Schematic of the custom dump-valve assembly installed in a spark-plug port.

A gas manifold (Figure 3) connects the dump valve to a 1-liter, Teflon-lined, stainless steel sample bottle and to a compact gas chromatograph (SRI Instruments Multi-Gas Analyzer #3). Pressure and temperature sensors instrument the manifold in order to monitor sampling events. Solenoid-operated isolation and vacuum valves deploy between sampling events to evacuate the manifold and minimize contamination by leaked gas. All manifold components are heated and insulated to maintain a temperature (90 °C) that is sufficient to avoid condensation of exhaust gases. The sequence of steps required to capture and analyze engine samples is described below in *Engine Operation and Sample Collection*.

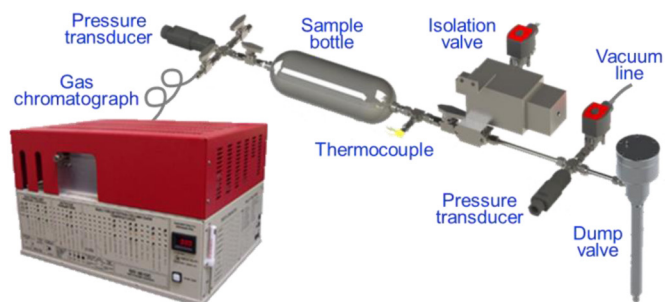


Figure 3. Arrangement of dump valve, gas manifold, sample bottle, and gas chromatograph.

The gas chromatograph (GC) houses three columns and detectors capable of speciating a wide range of molecules in the NVO gas samples. The first of two flame ionization detectors (FID #1) is connected to a 60-m capillary tube (Restek MXT-1) suitable for identifying intermediate and large hydrocarbons (HC). Sensitivity of the detector is high, providing low-noise measurements of C_3 to C_8 hydrocarbons.

A second FID (FID #2) and a thermal conductivity detector (TCD) are mounted in series on a pair of packed columns (2-m Restek Hayesep-D and 2-m Restek Molecular Sieve-13x). FID #2 is equipped with a methanizer that converts CO and CO_2 to methane in order to quantify the two gases. In addition, FID #2 is used to measure the C_1 - C_2 hydrocarbons that are insufficiently separated on the FID #1 capillary. For the current experiments, we switched the GC carrier gas from helium to nitrogen to make the TCD sensitive to hydrogen, potentially an important species for NVO research. In this configuration, the TCD quantifies concentrations of hydrogen, oxygen, and water.

Figure 4 presents the three chromatograms created by sending a single engine sample through the GC. Prominent peaks are marked with red horizontal line segments. Identification and calibration of the peaks requires sending multiple samples of known composition and concentration through the GC prior to the engine experiments. For the experiments presented here, a single-point calibration was used for each of the identified species. To extract a species concentration, the area beneath its peak is calculated and multiplied by the appropriate calibration factor. Based on repeated measurements,

uncertainty in reported concentrations is estimated to be better than $\pm 10\%$ for all but CO_2 which, for an unknown reason, exhibits greater scatter.

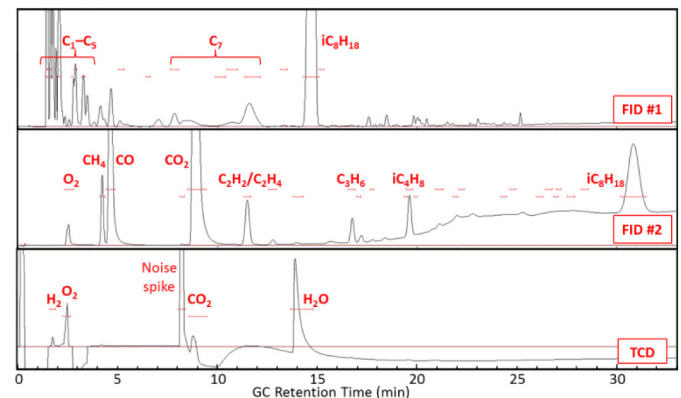


Figure 4. Sample chromatograms from the three GC detectors during a single GC run. Automated operation of the GC includes repeatably ramping carrier gas flows and temperatures to optimize separation of species. These events create noise spikes (which can be positioned to avoid species peaks) and variations in background that are easily removed during signal integration. Appearance of a small O_2 peak on FID #2 is an apparent artifact of the methanizer.

Certain species are not detected by FID or TCD, and others cannot be distinguished due to co-elution. To address this issue, several samples were transported to Lawrence Livermore National Laboratory (LLNL) for analysis on a GC equipped with a mass spectrometer. As an example, an important pair of species, acetylene and ethylene, co-elute on the Sandia GC, and they had to be separated at LLNL, as reported in the *Engine Simulation* section.

Engine Operation and Sample Collection

A single-cylinder engine configured for low-temperature gasoline combustion was used for the sampling experiments. The pent-roof head houses two intake valves and a single exhaust valve, providing room for a central, 8-hole, direct injector pointing vertically toward a flat-top piston. The head also includes two peripheral spark-plug ports. No spark plugs were used for the current experiments; instead, one spark-plug port housed the dump valve described above, and the second an embedded thermocouple to measure head surface temperature. For the current experiments, metal parts replaced all quartz components of this optical research engine.

Engine specifications and operating conditions used in the sampling experiments are listed in Table 1. The exhaust valve closing (EVC) and intake valve opening (IVO) events occurred 75 crank angle degrees (CAD) on either side of NVO TDC, thereby retaining a residual gas fraction of about 50%. The intake air temperature was elevated to enable compression-ignition operation at low load. To simplify sample gas speciation and facilitate modeling, iso-octane was selected as a surrogate fuel for gasoline. While holding injector trigger duration fixed, the injected mass of iso-octane diluted slowly, presumably due to variation in injector tip temperature. To